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By

Goang-Shin Liaw
Principal Investigator

ALABAMA A&M UNIVERSITY
Normal, Alabama 35762
Phone: (205)-851-5565
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SUMMARY

This report covers the research progress of NASA Grant NAG8-201 from May 1994 to August 1995. Four tasks were completed in this period and results were published in AIAA papers.

First, a Boltzmann-2D code, was developed and applied to compute MSFC-A2 nozzle/plume flow field. It solved the two-dimensional Boltzmann-BGK equation using the Finite Difference Discrete Ordinate (FDDO) numerical technique. The code was validated by experimental data for one-dimensional shock structure predictions, paper 95-2056. Successful results for nozzle/plume flow simulation using the developed Boltzmann-2D code were presented at the 1995 AIAA Aerospace Science Conference, paper 95-0627. Second, a computer code solving two-dimensional Burnett equations was developed and applied to low-density nozzle flow field calculation. Results were also published at the 1994 AIAA Thermophysics Conference, paper 94-2055. Third, the developed two-dimensional Burnett code was extended to compute axisymmetric flow field inside MSFC-A2 nozzle, paper 95-2008. The computed nozzle exit conditions are used as input data for Direct Simulation Monte Carlo (DSMC) plume calculation. Fourth, a DSMC code was modified to compute the exhausted plume near the nozzle exit and in the backflow region.

The published papers are listed as follows:

1. AIAA paper 94-2056: "Comparison of Shock Wave Structures by Solving Burnett and Boltzmann Equations";
2. AIAA paper 95-0627: "Numerical Investigations of Low-Density Nozzle Flow by Solving the Boltzmann Equation";
3. AIAA paper 94-2055: "Numerical Investigation of Low-Density Nozzle Flow Fields by Solving Navier-Stokes and Burnett Equations", AIAA 94-2055, 1994.
4. AIAA paper 95-2008: "Computation of Low-Density Axisymmetric Nozzle Flow Fields by Solving Burnett equations".

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1. INTRODUCTION

The objective of this research is to obtain accurate numerical solutions of a vacuum plume in the backflow region of a microthruster in orbital environments. As discussed in previous reports [1,2,3], the flow inside the nozzle is in the transitional regime and rapidly becomes rarefied in the plume and backflow region. In principle, the nozzle/plume flow fields are highly coupled. However, for first degree of approximation, it is reasonable to separate it into two independent flow fields: flowfield inside the nozzle and flowfield in the backflow region.

In this research, two approaches were used to compute the vacuum plume flowfield: the solution of the Boltzmann-BGK equation and the application of the DSMC technique.

Logically, the Boltzmann equation is the primitive governing equation for all non-equilibrium flows. Numerical solutions of the Boltzmann equation for fluid flows involve the calculation of the global molecular distribution function with the collision integral at each point in a three-dimensional infinite velocity space. It requires extremely long CPU time and large computer storage. To avoid these problems, it is common to solve more tractable Boltzmann-BGK equation. The advantage of solving the Boltzmann-BGK equation is that it requires much less computer time and still preserves the flow characteristics of the non-linear Boltzmann equation. In this research, a new computer code, which combines the FDDO technique [4,5] and the second-order upwind differencing scheme, was developed to solve the two-dimensional Boltzmann-BGK equation for the nozzle/plume flowfield.

Since the invention of the DSMC technique in early 1960's, it has been widely used to simulate the rarefied gas flow problems. The DSMC approach is an intuitive and probabilistic method which is capable of simulating the low-density and rarefied flows. Calculations can be made throughout the rarefied regimes and can overlap with the continuum calculations, the degree of overlap depends on the magnitude of the computation resources. Because the DSMC computational time is proportional to the number den-

sity in the computational domain, it is quite expensive to apply the DSMC method for the flowfield inside the nozzle. In this research, the DSMC technique is applied to the exhausted plume near the nozzle exit and the backflow region. The nozzle exit data, required by DSMC, are provided by the nozzle solutions. The nozzle exit flow conditions are very critical to the accuracy of the plume flowfield prediction since it affects the plume characteristics. Experimental data shows that the low-density flow inside the MSFC-A2 nozzle is in the transitional regime. However, the conventional Navier-Stokes equations cannot provide accurate solutions for flow in the transitional regime. Many research results demonstrated that the Burnett equations are more appropriate than the Navier-Stokes equations for transitional aerodynamic predictions [7,8]. Mathematically, the Burnett equations are one order higher than the Navier-Stokes equations in terms of the Chapmann-Enskog expansion. Its solution should capture more rarefaction effect in the transitional regime. In this research, the Burnett equations are solved for the flowfield inside the nozzle by modifying an existing continuum modeling technique. The goal of the code development for the Burnett equations is to provide an accurate nozzle exit conditions for the DSMC calculation.

2. ACHIEVEMENTS

2.1 Solving the BGK-Boltzmann Equation for Nozzle/Plume Flow

A new computer code, Boltzmann-2D, was developed to solve the two-dimensional Boltzmann-BGK equation for the nozzle/plume flow for MSFC-A2. It combines the FDDO and a second-order upwind differencing with the four-stage Runge-Kutta time integration technique to obtain steady state solutions. The solution procedure consists of three steps:

(1). Transforming the BGK-Boltzmann equation into two simultaneous partial differential equations by taking moments of the distribution function with respect to the molec-

ular velocity u_z, with weighting factors 1 and u_z^2.

(2). Solving the transformed equations in the physical space based on the time-marching technique and the four-stage Runge-Kutta time integration, for a given discrete-ordinate. The Roe's second-order upwind difference scheme is used to discretize the convective terms and the collision terms are treated as source terms.

(3). Using the newly calculated distribution functions at each point in the physical space to calculate the macroscopic flow parameters by the Modified Gaussian quadrature formula.

Repeating Steps 2 and 3 until the convergent criteria are reached. Detailed numerical formulation and solution procedures can be found in previous papers [9,10].

Low-density nozzle flow inside the MSFC-A2 and in its exhausted plume has been computed using the developed BGK-Boltzmann-2D code. The nozzle throat diameter is 0.054 inches with 20 degree half angle. The area ratio is 5.1. Figure 1 shows the nozzle configuration with the typical grids used in the Boltzmann-2D computation. The nozzle is placed between two reservoirs. The upstream and downstream boundaries of these two reservoirs are located about 15 times of the nozzle throat diameter from the nozzle inlet and exit respectively. Both upstream and downstream reservoir temperatures are set at 900 R with nozzle wall temperature equal to 540 R. The pressure ratio between the two reservoirs is 20:1. The Knudsen numbers are chosen as 0.1 and 1.0. It determines the upstream reservoir fluid density. Figure 2 shows the computed velocity vectors inside the nozzle for Knudsen number 0.1. Figures 3 and 4 show the Mach number contours inside the nozzle for Knudsen number 0.1 and 1.0, respectively. Each convergent solutions required about 8 hours of CPU time on the CRAY YMP. It clearly shows that the sonic line is shifted to the nozzle exit and substantial portions of the flow field inside the nozzle are subsonic. Figure 5 shows the Mach number distribution along the nozzle centerline. The comparison of the discharge coefficient between the solution of the Boltzmann-2D and the experimental data is shown in Figure 6. The discharge coefficient is defined by

taking the ratio of the Boltzmann-2D mass flow rate to the one-dimensional theoretical value at the same Knudsen number and Reynolds number. Both the Knudsen number and the Reynolds number are defined in terms of the nozzle throat diameter. Reasonable agreement was found at $K_n = 1.0$. At $K_n = 0.1$, results do not match well with experimental data. The discrepancy is probably due to the two-dimensional nature of this Boltzmann-BGK code, while the experimental data were obtained from the conical nozzle. For larger Knudsen number, Boltzmann-2D solutions converges faster.

2.2 Code Development of Two-Dimensional Burnett Equations

As a first step to obtain nozzle exit conditions, a computer code, Burnett-2D, to solve the two-dimensional Burnett equations has been developed. It extends the RPLUS2D code to implement high-order Burnett source terms and slip-wall conditions for velocity and temperature. The Burnett-2D code employs finite volume, upwind lower-upper time marching techniques. High-order Burnett viscous stress and heat flux terms were discretized using central-differencing and treated as source terms. Slip-wall conditions for both velocity and temperature were treated implicitly. The detailed numerical formulations and solution procedures can be found in Deng [11].

A two-dimensional nozzle has been selected for the calculation. This nozzle has an area ratio of 11.40 with a 12.833 degree half angle at the nozzle exit. The ratio of the nozzle axial length to the throat diameter is 15.32. The nozzle throat diameter d_{throat} is $5mm$. The chamber pressures are chosen at $0.1, 0.25, 0.5$ and $1.0psi$. The chamber temperature is $2025K$ for all calculations. Two types of boundary conditions are specified on the nozzle wall: no-slip with adiabatic wall and slip with isothermal wall.

Figures 7(a), 7(b) and 7(c) show the Burnett solutions of velocity vectors, local Mach number and averaged Knudsen number contours with chamber pressure 0.1 psi, under adiabatic wall conditions. In this case, the calculated Reynolds number based on the nozzle throat diameter is 40. The averaged Knudsen number with respect to nozzle

throat diameter, ranges from 0.03 at nozzle inlet to 0.3 at nozzle exit, which indicates that the nozzle flow field is in the transitional regime. A decelerating region is found near the nozzle centerline from the Mach number contours in Figures 7(b).

Burnett equations are also solved with the slip-wall boundary conditions. The wall temperature is constant. The nozzle chamber pressures are $0.1, 0.25, 0.5$ and $1.0psi$. The chamber temperature is 2025 K. The wall temperature is 300 K for all calculations. Figure 8 shows the comparisons between the solutions of Burnett and Navier-Stokes equations for nozzle centerline Mach numbers at different chamber pressures of $0.1, 0.25$ and $1.0psi$, respectively. At chamber pressure of $0.1psi$, the Knudsen number at the wall ranges from 0.002 to 0.02. In this case, a slight difference can be found in the centerline Mach number and nozzle exit velocity.

2.3 Axisymmetric Flow Solver and MSFC-A2 Nozzle Exit Conditions

For predictions of low-density nozzle flow field, it is necessary to develop a two-dimensional axisymmetric flow solver. As a second step to obtain accurate nozzle exit conditions, the previous Burnett-2D code was extended to Burnett-2DAX code, which solves axisymmetric flows for a low-density nozzle. After the axisymmetric formulations of the high-order Burnett stress and heat flux components have been derived, the axisymmetric Burnett terms are implemented into the Burnett code as source terms.

The flow field inside the MSFC-A2 nozzle was computed using the developing Burnett-2DAX code. Three chamber pressures were selected in order to compare the results with available experimental data and DSMC solutions. The chamber pressures are chosen at $516.4, 303.4$, and $175.3Pa$. The chamber and wall temperatures are fixed at $270K$ for all calculations. Constant nozzle wall temperature and slip-wall conditions are applied. The averaged Knudsen number is calculated in terms of the nozzle throat diameter,

$$Kn = \frac{\lambda_1}{d_{throat}} = \frac{16}{5d_{throat}} \frac{\mu}{\rho\sqrt{2\pi RT}}$$

The calculated pseudo-Reynolds number,

$$R_e^* = \frac{4\dot{m}}{\pi d_{throat}\mu_0} = 24.26,$$

is based on the nozzle throat diameter d_{throat} and viscosity at chamber conditions, μ_0. The maximum Knudsen number is found near the nozzle exit. These axisymmetric nozzle solutions are significantly different from those of two-dimensional nozzle calculations, where the maximum Knudsen number was found near the nozzle wall. As shown in Figures 9, the flow is highly viscous and a "supersonic bubble" is clearly observed inside the nozzle. This phenomenon is similar to the experimental observations. Figure 10 shows the Burnett solutions of Mach number distribution along the nozzle axis for two chamber conditions. The flow is not choked at the throat for either cases.

As the chamber pressure decreases, the pseudo-Reynolds number decreases. The averaged Knudsen number increases, and the flow inside the nozzle becomes more rarefied. Using the developed axisymmetric Burnett code, Table 1 summarizes the computed mass flow rate and discharge coefficient C_d. The nozzle discharge coefficient is calculated based on

$$C_d = \frac{\dot{m}}{\dot{m}_{isentropic}}$$

where $\dot{m}$ is the calculated nozzle mass flow rate, and $\dot{m}_{isentropic}$ is the one-dimensional isentropic nozzle mass flow rate.

Table 1. Burnett C_d

$P_0(Pa)$	$\dot{m}(\times 10^7 kg/s)$	Re_*	C_d
175.3	0.8154	4.14	0.3244
303.4	2.2142	11.24	0.5074
516.4	4.7805	24.26	0.6433

Figure 11 shows the comparison of nozzle discharge coefficient versus pseudo-throat-Reynolds number among Burnett, DSMC solutions and experimental data. The DSMC solutions and experimental data for MSFC-A2 nozzle were adopted from Brewer [13]. The axisymmetric Burnett solutions were found in good agreement with experimental data as well as DSMC solutions when pseudo-throat-Reynolds number is greater than

10, where the flow inside the nozzle is in the transitional regime. This indicates that the Navier-Stokes solutions are not applicable. The merit of adopting the Burnett equations as the governing equations is that all the numerical methods for continuum flows are applicable. The solution of Burnett equations requires much less computer resources compared to the application of DSMC technique. However, the Burnett solutions begin to deteriorate when pseudo-throat-Reynolds number is below 10, where the flow inside the nozzle is highly rarefied. This discrepancy may come from the formulations of slip-wall conditions. As the nozzle flow field becomes more rarefied, more appropriate slip-wall conditions or other wall-treatment are needed.

Detailed description of the formulations of axisymmetric Burnett terms, numerical procedure and results on MSFC-A2 nozzle computation can be found in Deng [12].

The computed nozzle exit conditions, which include velocities, Mach number, temperature, Knudsen number and pressure are used as input data for DSMC simulations. Figure 12 shows the distributions of nozzle exit velocity and Mach number for the MSFC-A2 nozzle, at chamber pressure 303 Pa and chamber temperature 270 K. Constant temperature with slip-wall conditions were applied at the nozzle wall.

2.4 DSMC Solutions for Plume in the Backflow Region

The DSMC solutions for plume flowfield near the MSFC-A2 nozzle exit and in the backflow region of the nozzle were obtained using Bird's G2 code [6]. The plume flowfield is assumed to be two-dimensional axisymmetric. The computational domain is illustrated in Figure 13. The nozzle exit conditions were calculated prior to the Burnett-2DAX code. The nozzle chamber pressure is 303 Pa, and the nozzle chamber temperature is 270 K. Constant wall temperature was assumed. The inflow boundary is at the nozzle exit. As to other boundaries, the vacuum condition is employed, and there is no mass transfer across these boundaries. Preliminary results for velocity streamline and density contours are plotted in Figures 14. The exhaust plume in the backflow region is clearly visualized

and the plume flowfield is highly rarefied.

3. FUTURE WORK

The Boltzmann-2D code will be applied to compute nozzle/plume flows. The boundary conditions will be carefully investigated. The DSMC method will be used to compute vacuum plume in the backflow region.

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Low-Density Nozzle Flow by Solving the Boltzmann Equation", AIAA 95-0627, 1995.

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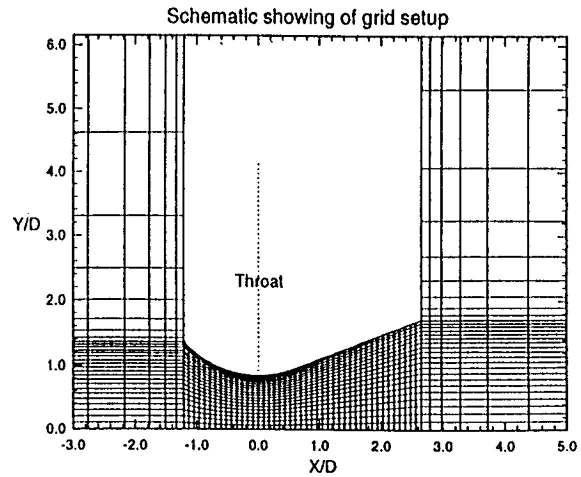


Figure 1. Grid setup for Boltzmann-2D nozzle/plume simulation.

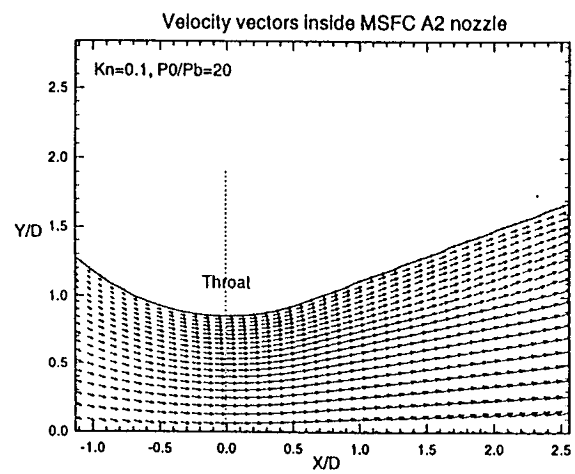


Figure 2. Velocity vectors inside the nozzle for Kn=0.1.

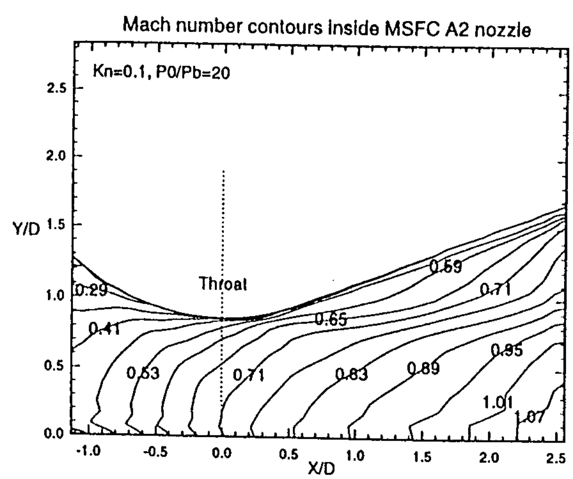


Figure 3. Mach number contours inside the nozzle for Kn=0.1.

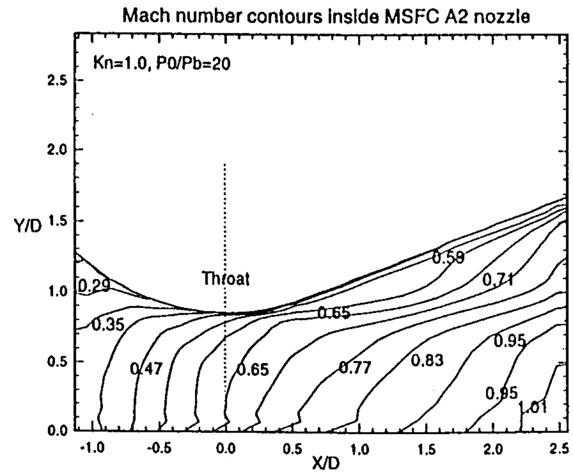


Figure 4. Mach number contours inside the nozzle for Kn=1.0.

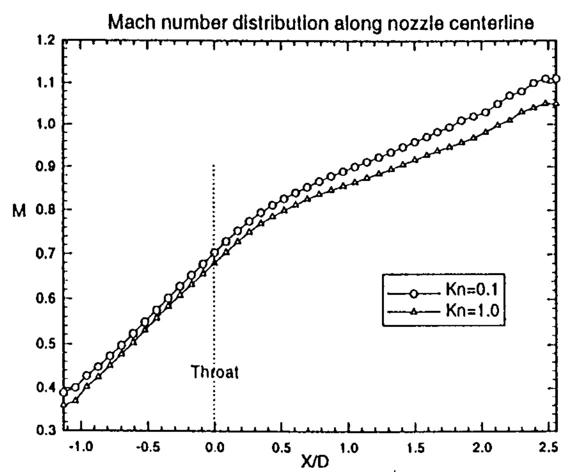


Figure 5. Mach number distribution along nozzle axis.

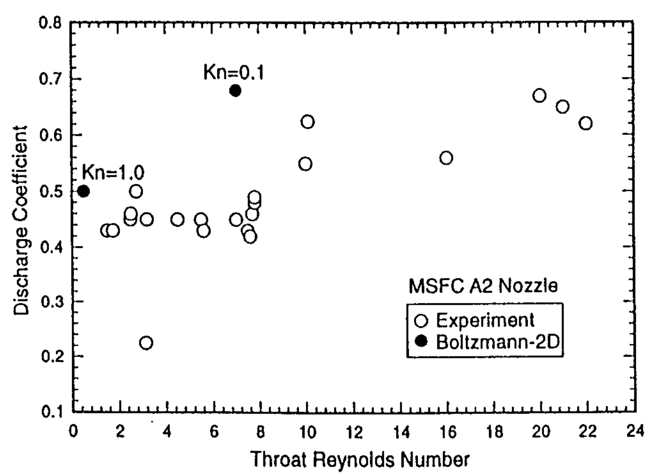


Figure 6. Comparison of calculated discharge coefficient with experiment.

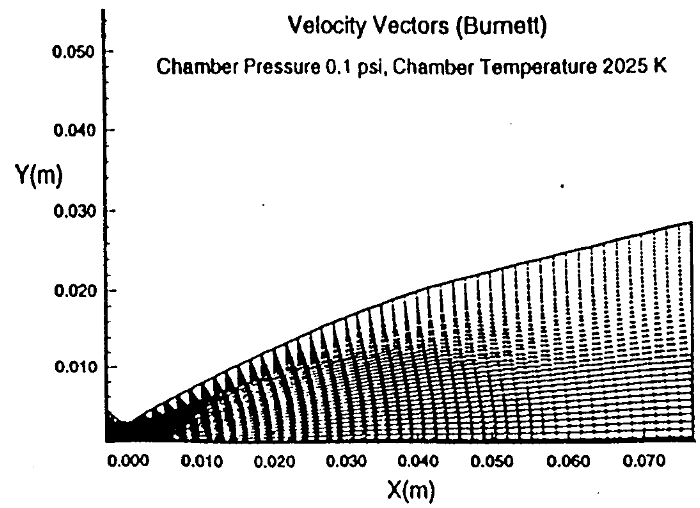


Figure 7(a). Burnett-2D velocity vectors. Adiabatic wall.

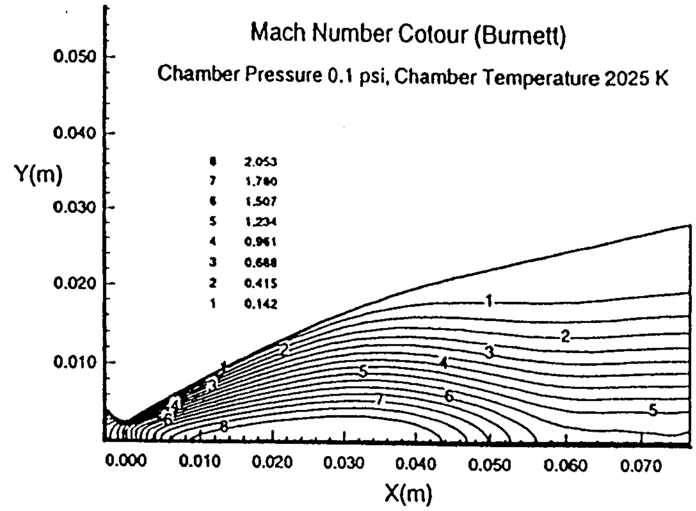


Figure 7(b). Burnett-2D Mach number contours. Adiabatic wall.

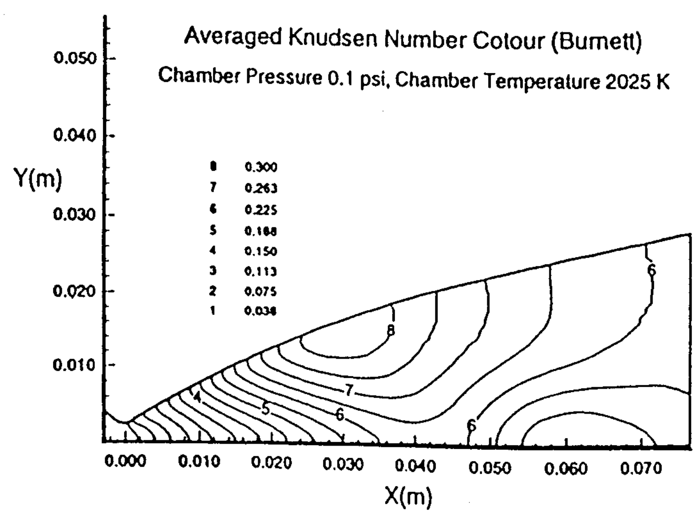


Figure 7(c). Burnett-2D Knudsen number contours. Adiabatic wall.

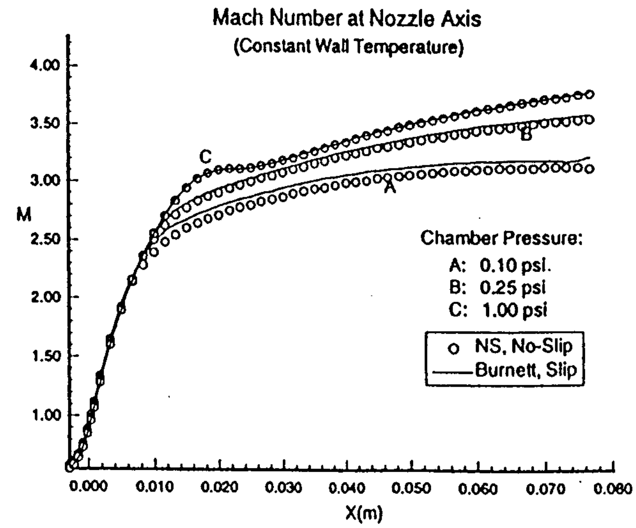


Figure 8. Burnett-2D: Nozzle centerline Mach number comparison.

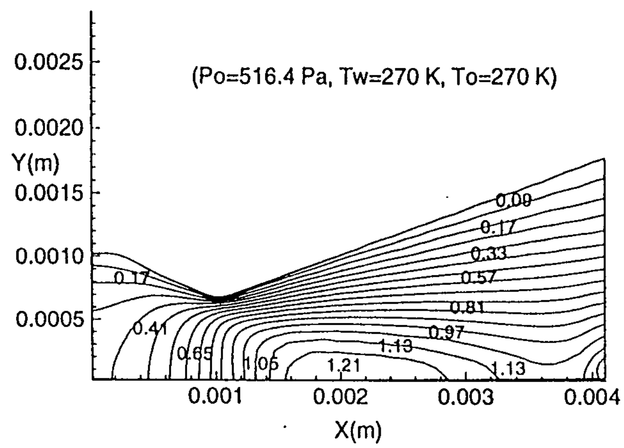


Figure 9. Burnett-2DAX: Mach number contours. Slip-wall, constant wall temperature.

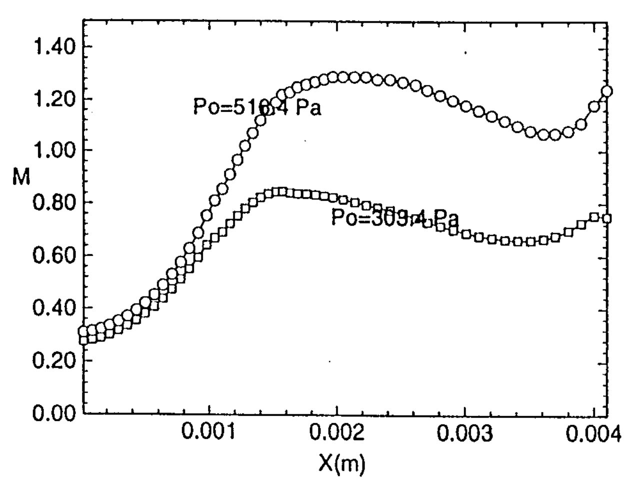


Figure 10. Burnett-2DAX: Mach number along centerline.

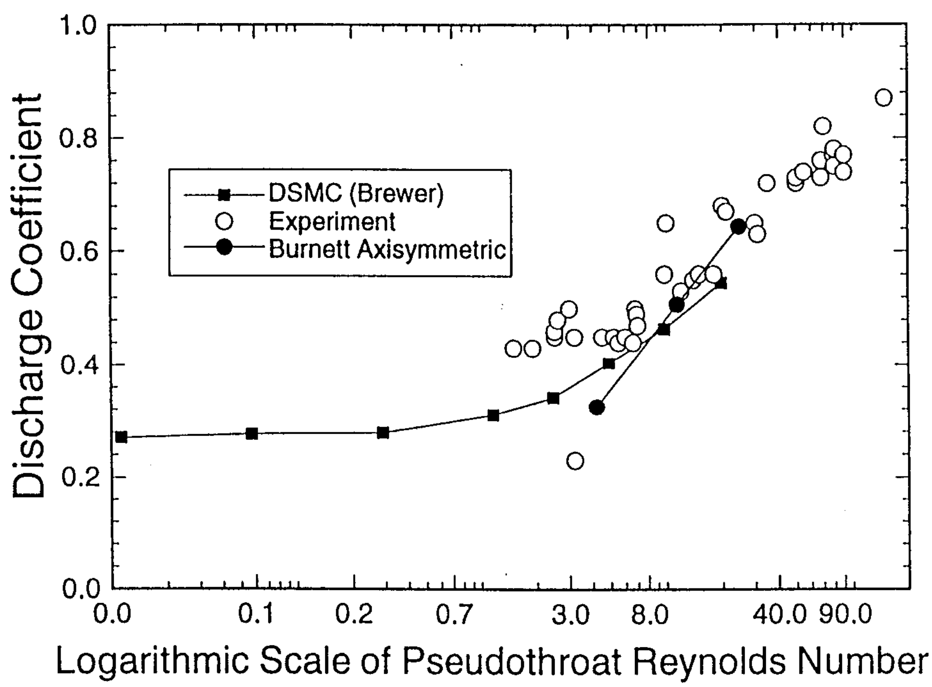
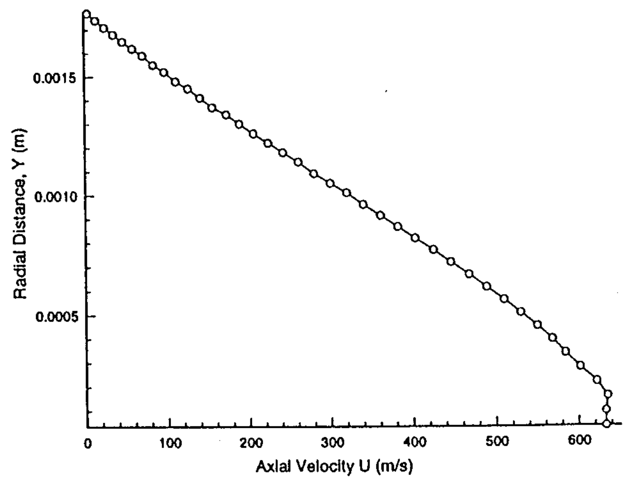
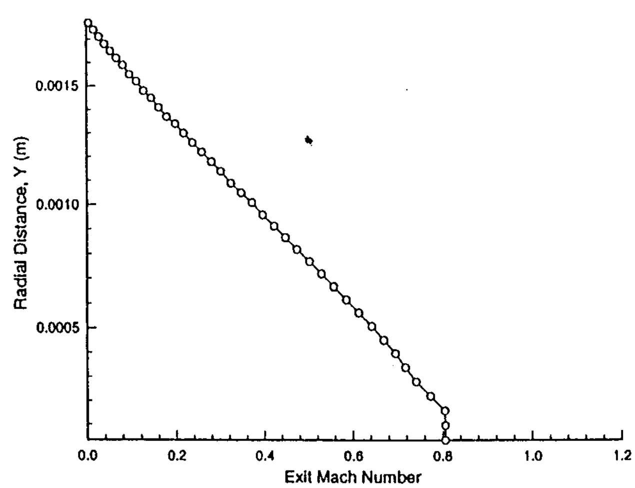


Figure 11. Comparison of discharge coefficient with DSMC and experimental data.



(a). Exit Velocity Distribution



(b). Exit Mach Number Distribution

Figure 12. Burnett-2DAX solution of MSFC-A2 nozzle flowfield.

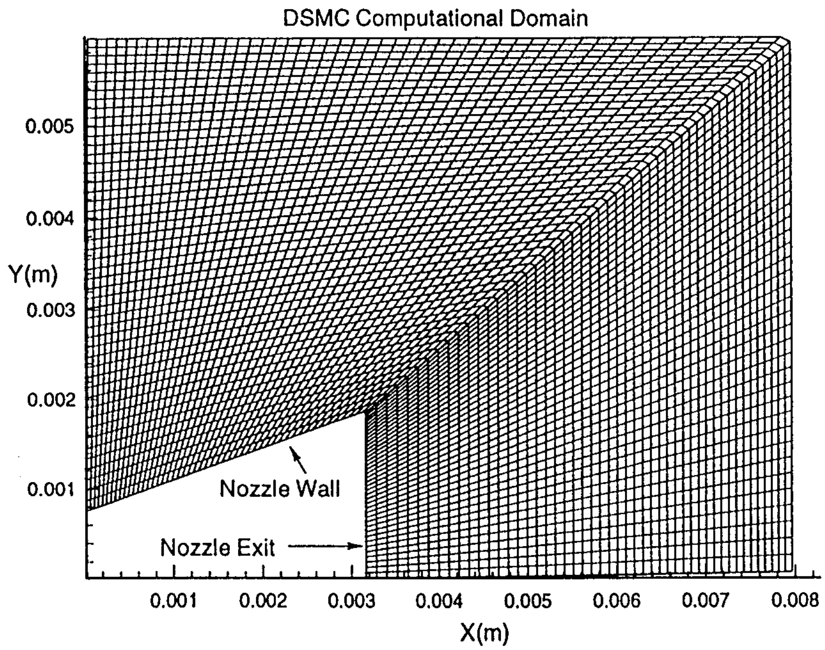


Figure 13. DSMC domain configuration.

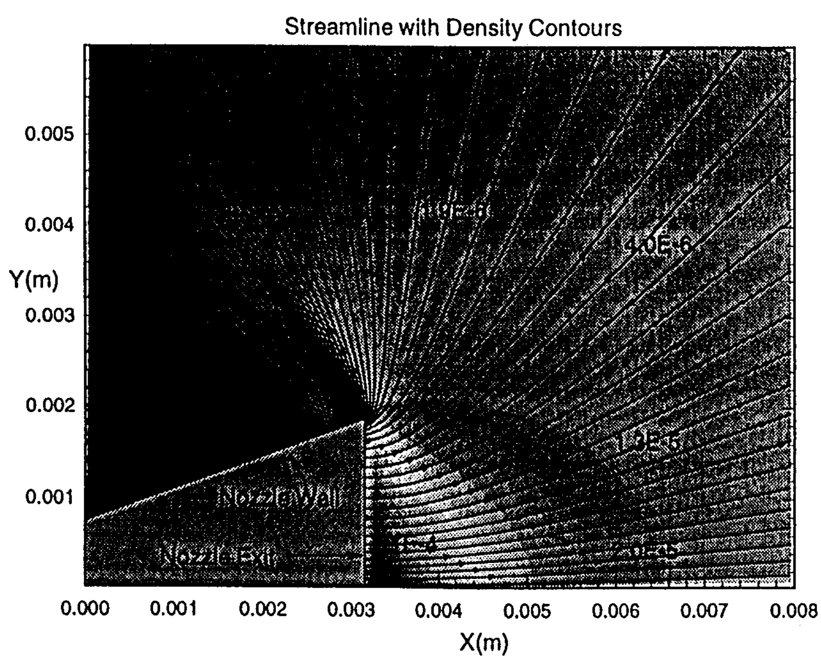


Figure 14. DSMC streamline and Density contour.